

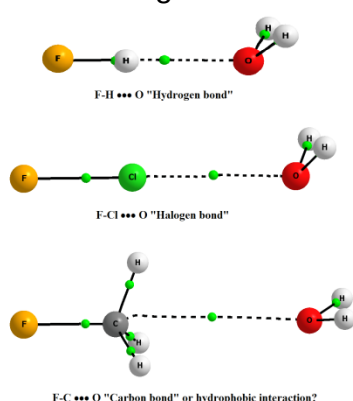
Molecular Beam Microwave Spectroscopy: Defining Hydrogen Bond and Discovering Carbon Bond!

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Hydrogen bonding was postulated in the early 20th century based on the stunning macroscopic differences between the first and second row hydrides i.e. water is a high boiling liquid without which there would be no life and hydrogen sulphide is a stinking gas, under ambient conditions.^[1] Our laboratory has been investigating a series of H₂O and H₂S complexes using molecular beam microwave spectroscopy and advance theoretical methods and showed that both H₂O and H₂S can form hydrogen bonds.^[2] This and other developments led us to initiate and complete an IUPAC project to redefine hydrogen bonds.^[3] We have just given the direct experimental confirmation that H₂S dimer is hydrogen bonded based on its well resolved microwave spectrum.^[4]

Our recent work on the unremarkable Argon-propargyl alcohol complex suggested that there might be Ar---C interaction in addition to the expected O-H---Ar interaction in this complex.^[5] This eventually led us to define a 'carbon bond' analogous to the 'hydrogen bond'.^[6] As an example, atoms in molecules theoretical studies reveal a bond critical point connecting O of H₂O to the C of CH₃F (See Figure). This interaction would have been thought of as the 'hydrophobic interaction', which is an ill-defined term. Over the



last few decades, chemists have identified halogen bonding (group 17)^[7], chalcogen bonding, (group 16)^[8] and pnicogen bonding (group 15)^[9]. We are pleased that this could be extended to group 14 and the most important element in the periodic table, carbon. Our prediction of the 'carbon bond' has been experimentally verified by spectroscopy^[10] and crystallography^[11]. Clearly the "periodic table of intermolecular bonding" also began with "hydrogen" bonding.

References

- [1] L. Pauling, *Nature of Chemical Bond*, Cornell University Press 1960 Edition.
- [2] M. Goswami and E. Arunan, *Phys. Chem. Chem. Phys.* **2009**, *11*, 8974.
- [3] E. Arunan, G. R. Desiraju, R. A. Klein, J. Sadlej, S. Scheiner, I. Alkorta, D. C. Clary, R. H. Crabtree, J. J. Dannenberg, P. Hobza, H. G. Kjaergaard, A. C. Legon, B. Mennucci and D. J. Nesbitt, *Pure Appl. Chem.*, **2011**, *83*, 1619 & 1637.
- [4] A. Das, P. K. Mandal, F. J. Lovas, C. Medcraft, N. J. Walker, and E. Arunan, *Angew. Chem. Int. Ed. Engl.* **2018**, Accepted for publication.
- [5] D. Mani and E. Arunan, *ChemPhysChem* **2013**, *14*, 754.
- [6] D. Mani and E. Arunan, *Phys. Chem. Chem. Phys.* **2013**, *15*, 14377.
- [7] P. Metrangola and G. Resnati, *Chem. Euro.J.* **2001**, *7*, 2511-2519.
- [8] D. Manna and G. Mugesh, *J. Am. Chem. Soc.*, **2012**, *134*, 4269-4279.
- [9] S. Scheiner, *J. Chem. Phys.*, **2011**, *134*, 094315-094319.
- [10] S. A. Southern and D. L. Bryce *J. Phys. Chem. A*, **2015**, *119*, 11891–11899.
- [11] S. P. Thomas, M. S. Pavan and T. N. Guru Row, *Chem. Comm.* **2013**